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FRICTIONAL HOT-SPOTS AND STATISTICAL CRACK MECHANICS

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ABSTRACT

When propellant cylinders are fired at low speeds against a steel plate, detonations are often observed. Since the process is not repeatable, and shock heating is not significant, it is natural to consider the possibility of detonation caused by hot spots. Several mechanisms are compared, and it is suggested that interfacial friction of closed cracks seems to be the most likely mechanism.

INTRODUCTION

There is always a risk of structural failure in solid propellants, but under some circumstances the failure culminates in a violent explosion. Thus, the usual structural problems of solid propellants are exacerbated by the possibility of additional damage from detonations. In addition, solid propellants are sensitive to the rate of loading. In a series of experiments reported by Jensen, Blommer and Brown [1], test cylinders of propellants were fired against a steel target plate using a 12-gauge shotgun, and it was found that for impact velocities above 300 m/s reactions fell into three categories. Above 800 m/s, violent reactions occurred shortly after impact, which were designated as SDT (Shock to Detonation Transition). But below 800 m/s about 76% experienced a mild deflagration (DEF), while the remaining 24% reacted violently at relatively late times after impact (XDT), with the X designating an unknown etiology. A paper by Green et. al. [2] describes similar results involving larger cylinders of propellant impacted by steel cylinders. That work shows a systematic reduction in threshold velocity with increasing speed.

In order to explain the erratic character of the detonation it seems natural to consider hot-spot mechanisms associated with flaws in the propellant. The occasional occurrence of flaws exceeding a critical size would explain the lack of repeatibility, while the increasing number of flaws with sample size would explain the reduction in threshold velocity with increasing sample size. If the hot-spot explanation is to be explained quantitatively, however, it is necessary to consider specific mechanisms. Though experiments are fundamental, it is difficult to control and observe hot-spot behavior on the scale of a few microns. Thus, theoretical analysis of these problems appears as an interesting alternative.

Four hot-spot mechanisms seem to be the most likely candidates for explaining XDT; void collapse with closing shock; void collapse with plastic flow; shear banding with plastic flow; and shear cracking with frictional heating. These mechanisms will be considered separately in the sections that follow. The frictional heating mechanism seems to be the most important in connection with XDT, and explains the observed phenomena, but hot spots with more complex geometries and mechanisms than those considered so

far may well be important, and better analyses could alter the conclusions drawn here.

Continuum theories have also been proposed to describe XDT. Hydrodynamic calculations involving rarefaction and recompaction are described in [2], as well as flash radiographs showing low density zones. Jacobsen and Karpp [3] describe continuum calculations using a continuum reaction law, and support the rarefaction and recompaction mechanism for XDT. Explanations of a continuum type, however, cannot explain why only a small fraction of identical shots lead to XDT, nor is much information provided about how material properties and flaw structure may affect propellant sensitivity

A statistical treatment of material properties offers a number of advantages. In the statistical crack mechanics work at Los Alamos we consider the strain rate of a solid to be the sum of strain rates associated with continuum and flaw deformations. The method has its conceptual origins in the NAG-FRAG work at Stanford Research Institute [4], but our statistical crack mechanics algorithms differ in detail and, in particular, do not make use of the iterative procedures implicit in the SRI formulations, and thereby avoid convergence difficulties. The strain rates associated with the opening, shear, growth and coalescence of crack are accounted for by separate constitutive theories. The result is a constitutive law characterizing a fragmenting solid, for which details are given in the review by Dienes [5], and a summary is provided at the end of this paper. For the analysis of XDT, a peak temperature at the center of a sliding crack is computed from frictional heating, and that determines the possibility of ignition [6]. The statistical character of the result arises from the distribution of crack sizes, which can be used to estimate the maximum crack size occurring in each portion of the test sample.

VOID COLLAPSE WITH SHOCK HEATING

When a cylinder of propellant strikes a steel plate, a shock is propagated along its length, while a rarefaction wave propagates in from the surface of the cylinder behind the shock, releasing the pressure. Still, the pressure remains high in the interior for a significant time. Numerical solutions of such problems can be obtained, providing a suitable description of material behavior is known, but in this article a comparison of various heating mechanisms is made by order-of-magnitude arguments. The shock heating can be estimated using an approximate theory described in the appendix. To accomplish this the compression is computed from the standard shock relation

$$\theta_s = \frac{\rho - \rho_0}{\rho} = \frac{u}{u + u_s} \quad , \tag{1}$$

where ρ_0 and ρ are the initial and shock densities, u is the velocity of impact against the steel plates, considered rigid, and u_s is the shock speed, which can be taken as equal to the sound speed, c_0, for moderate shocks. The shock pressure can be estimated from the Hugoniot relation

$$P_s = \frac{A}{W}\,\frac{e^{W\theta_s} - 1}{1 - G\theta_s/2} \quad , \tag{2}$$

where G is Gruneisen's ration; W, a material constant on the order of 5; and A is the bulk modulus

$$A = \rho_0 c_0^2 \quad . \tag{3}$$

In this approximate analysis the effect of shear is neglected. Though often a reasonable approximation, it is extremely good for propellants, which tend to be rubbery, and for which a typical Poisson's ratio is $\nu = 0.49$. (The reader is reminded that 0.3 is typical for many materials, and 0.5 denotes an incompressible material.) The specific internal energy increment for the shocked material is

$$I_s = \frac{1}{2} p_s V_0 \theta_s \quad , \tag{4}$$

and the temperature rise, using the same approximation, is given by

$$C_v \Delta T_s = I_s - \frac{A/\rho_0}{W - G}\left(\frac{e^{W\theta_s} - 1}{W} - \frac{e^{G\theta_s} - 1}{G}\right) \quad . \tag{5}$$

It also follows from the appendix that for material expanding adiabatically behind a shock

$$\Delta T = \Delta T_s \, e^{G(\theta - \theta_s)} \quad . \tag{6}$$

For a typical propellant $\rho_0 = 2000$ Kg/m^3, $c_0 = 2000$ m/s $G = 2$, $W = 5$, and $C_v = 1460$ J/Kg. At the lower limit for XDT, $u = 300$ m/s, it follows that $\theta_s = 0.13$, $p_s = 1.7$ GPa, $I_s = 55$ KJ/Kg and $\Delta T_s = 5.9$°C, where the subscript s denotes a value behind the shock. This temperature rise is not sufficient to have any effect. At 1000 m/s, a speed at which SDT is systematically observed, $\theta_s = 0.33$, $p_s = 10.3$ GPa, $I_s = 858$ KJ/Kg, and $\Delta T_s = 236$°C. This temperature rise is enough to ignite grains of HMX 385μ in thickness, using the theory of Frank-Kamenetskii [8] and data of Rogers [7]. Since propellants are about 50% HMX, and the binder is reactive, it is not surprising that SDT was observed at this speed in the samples tested by Jennings, Blommer and Brown [1], which are 17 mm in diameter. The effect of adiabatic expansion to $\theta = 0$ is to reduce the temperature increment for the low speed impact from 5.9°C to 4.5°C, and for the high speed impact to reduce the temperature increment from 236°C to 115°C. In the low-speed case, the effect is negligible, while for the high-speed impact the effect is significant if the time scale is of the same order as the ignition time. This detail depends on the size of the projectile and the sensitivity of the explosives.

If voids exist in the shape of thin ellipsoids, shock pressure will cause them to close at a speed slightly above the original projectile speed. At closure, shock heating will cause a temperature rise slightly higher than that associated with projectile impact. At 300 m/s, this is still not enough to be important (under 12°C), but at 1000 m/s the secondary shock will bring the temperature rise over 400°C, enough to initiate a reaction rapidly. Additional information on the effect of temperature on reaction rates will be mentioned in connection with frictional heating. In

this section the point is only to indicate that void closure is unlikely to be responsible for XDT in the neighborhood of 300 m/s. Though under some conditions jets may form during void collapse, the associated temperature rise is probably still unimportant.

VOID COLLAPSE WITH PLASTIC FLOW

Void collapse in a solid is accompanied by energy dissipation, which depends on material properties and void geometry. In order to estimate the associated temperature rise it is convenient to assume spherical collapse and an ideally plastic, isochoric (incompressible) material. It is straightforward to show that the shear strain at the surface of such a void collapsing from an initial radius a_0 to a current radius a is $\sqrt{3}\ \ell n\ (a_0/a)$. Then the temperature rise on the surface of the void, in the absence of conduction, is

$$\Delta T = \frac{\sqrt{3}\ Y}{\rho C_v}\ \ell n \left(\frac{a_0}{a}\right) \quad . \tag{7}$$

The additional closure resulting from thermal expansion is sufficient to close the void, to a rough appoximation, when

$$\frac{4}{3}\ \pi\ a^3 = \frac{4}{3}\ \pi\ a_0^3\ \ \alpha\Delta T \quad , \tag{8}$$

where α is the volume coefficient of expansion. The peak temperature rise at collapse is given, in this approximation, by the solution to the transcendental equation

$$\theta = \beta\ \ell n \left(\frac{1}{\theta}\right) \quad , \tag{9}$$

where

$$\theta = \alpha\Delta T, \quad \beta = \frac{Y\alpha}{\sqrt{3}\ \rho\ C_v} = \frac{YG}{\sqrt{3}\ A} \quad . \tag{10}$$

Taking Y = 10 MPa, and values of G and A given above, $\beta = 0.00289$. Then, $\theta = 0.0126$, and using the value $\alpha = 0.00073$ that follows from $\alpha = GC_v/c_0^2$, it follows that $\Delta T = 17°C$. This temperature rise is insufficient to result in a significant reaction, especially when the small mass of material involved in typical voids is considered. A significant role for this process in XDT is made still more unlikely when the effect of thermal softening, which reduces the flow stress as the temperature rises, is considered.

SHEAR BANDING

The shear banding instability arises when the heating due to shear stresses reduces the strength of a material in such a way as to localize the region in which shearing and heating occur. This effect is important

in the high speed deformation of metals, and it is of particular interest in connection with the high speed deformation of propellants since the heating can be enhanced by the reactivity of the material. The problem has been studied by Frey [9] using numerical integration of the heat equation with mechanical and chemical heat sources. He does not, however, make use of the momentum equation and, hence, does not actually represent the mechanical instability. (An elegant analysis of the mechanical stability problem has recently been reported by Bai [10], and it would be of interest to extend his analysis to include the effect of chemical heating.) The approach to melting as a result of shear stresses can be estimated by computing the temperature rise in time t (in the absence of a chemical contribution) from the simple relation

$$\Delta T = \frac{Y\dot{\varepsilon}t}{\rho C_v} \quad . \tag{11}$$

Using previous estimates of these variables, one finds that in 1 μs the temperature rises 0.4°C for a strain rate of 10^5 s^{-1}. This heating proves small in comparison with the frictional process described in the next section.

FRICTIONAL HOT SPOTS

The heating of a closed crack associated with interfacial sliding can be estimated from the solution to the one-dimensional heat flow equation

$$\Delta T = 2\dot{Q}\sqrt{t/\pi k\rho C_v} \quad , \tag{12}$$

where $\dot{Q} = \mu\sigma v$ is the surface heating due to friction, with μ the coefficient of friction, σ the normal stress, and v the sliding velocity. Taking $\mu = 1$, $\sigma = 1$ GPa, $k = 0.43$ J/m/K/s, and the sliding velocity as 1 m/s, one finds $\Delta T = 994$°C in 1 μs. The melting point of HMX at a pressure of one GPa is estimated as about 480°C, assuming a slope for the melting curve of 200 K/GPa, typical of organic materials [9], and a melting point for HMX under normal conditions of 280°C [11]. It is proposed that this very rapid temperature rise is the controlling process in XDT. At melting, the heat removed from the crack by conduction must just balance the heat produced by the interfacial stress. Thus, it is assumed that the stress state at a crack surface is governed by the thermal properties of the material. The material at the crack surface is, then, in transition between the solid and liquid states.

I have calculated the time to ignition for HMX with a surface held at 480°C to be 50 μs [6] using the Arrhenius law and physical constants determined and verified by Rogers [7]. The calculation involves numerical integration of the Poisson-Boltzmann equation

$$\dot{T} + DT_{xx} = \alpha e^{-Q/kT} \quad , \tag{13}$$

for a semi-infinite solid rounded by a plane held at a fixed temperature, T_m. The calculation, which is done implicitely, indicates a sudden development of very high temperature when heat conduction is no longer capable of removing a significant part of the heat produced chemically. The actual

process of XDT may well be more complex than the one described here, which involves simple estimates of crack behavior. In reality, crack behavior is very complex even in simple materials, and even more complications can be expected in propellants, which are heterogeneous mixtures of rather peculiar constituents.

In a complete description of XDT it would be necessary to describe both the mechanical behavior of flaws and the transient loading they are subjected to. This is clearly difficult, since the flaws themselves influence the environment of their neighbors. An approach to this problem is described by Dienes [5], which involves formulating a constitutive law that accounts for the opening, shear, growth and coalescence of cracks. A detailed discussion is beyond the scope of this paper, and only a few salient points are outlined herein. The problem is to write a constitutive law, suitable for numerical integration, that describes the main features of a fragmenting material. In general, two lines have been adopted, which can be described as the continuum and the statistical. In the former, phenomenological laws that are typically generalizations of visco-elastic-plastic theory are hypothesized [12], while in the latter material response is considered as a superposition of effects, including particularly the influence of flaws. As mentioned above, the latter approach is taken at SRI [4], where correlation of numerical results with tests is emphasized; by Kachanov [13], who has explored the theoretical foundations; and in the current work. (No effort is made here to review all the work involving statistical approaches.) Advantages of the statistical approach are that it can account for size and rate effects, which are important in fragmentation [12,15], and it becomes possible to characterize the most important underlying physical processes. In the application to propellant sensitivity this is particularly important because of the need to account for chemical reactions involving very small dimensions.

Explicit expressions for the strain rates due to matrix distortion, crack opening and crack shear [5], each involving the product of a compliance matrix and the stress rate, are superposed to obtain the elastic contribution. Care must be taken in formulating the stress rate to account for material rotation which can influence the components of stress while the physical state remains unaltered. A theory for carrying out the calculation valid for large deformations, described by Dienes [16], generalizes the small deformation theory of Noll [17] and avoids a potential instability of Noll's theory at large strains. In addition to these contributions to the stress rate, which are essentially elastic in nature, there is a contribution due to crack growth that is essentialiy nonlinear, since the growth depends on the stress level. Growth is said to occur when the stress exceeds a critical level, and growth for each crack orientation must be considered separately. It is also necessary to consider the stability of open and closed cracks separately, with interfacial friction acting as a stabilizing mechanism in the case of closed cracks. In addition to instability, it is necessary to consider whether closed cracks are locked by friction, and the dissipation effect of friction if cracks are not locked. In initial work on this problem [15,18] the effect of interfacial stresses on stability and deformation was not adequately accounted for, but the corrections have been made [5] and the effect on numerical results proves to be small. Strain rates due to viscosity and the effects of high pressure are readily incorporated into the formalism.

The constitutive relation depends strongly on the statistical distribution of flaws $\mathcal{N}(c, \Omega, t)$, with the dependence on c respresenting the effect of crack size, the dependence on Ω representing the effect of crack

orientation, and the dependence on t representing the effect of crack growth. The distribution is taken to be the sum of the distribution of isolated cracks $\mathscr{L}(c, \Omega, t)$ initially present in the material, and connected cracks $\mathscr{M}(c, \Omega, t)$ that have encountered enough other cracks to terminate this growth. In initial work on this problem [19] it was assumed that the rate of crack growth and the mean free path of cracks (before encountering other cracks) are constant, but a theory has recently been developed that accounts for variations in crack speed with stress level, and mean free path with crack size [5].

The permeability of solids depends on the number of connected cracks, and is independent of the isolated cracks, except insofar as they create confusion in understanding the crack structure of actual materials. It is important in computing the permeability of materials to account for the effect of percolation theory [20], which makes it possible to find the fraction of connected cracks that are isolated in the larger sense of not belonging to an infinite path. Current SCRAM calculations allow for a calculation of permeability, though its reliability has still not been established.

Calculations of a cylinder of propellant impacting a steel plate have been carried out using the algorithms of statistical crack mechanics [6], and we find that at 300 m/s closed cracks remain at the melting point for just 50 μs, the time required for ignition at an ambient pressure of one GPa. This provides encouragement that the frictional hot spot is the mechanism underlying XDT, though more work is required before definitive results can be claimed.

APPENDIX

The equation of state of solids at high pressure has been studied extensively at Los Alamos, and results have been published for many materials, beginning with the paper of Walsh and Christian [21]. A relatively complete summary is given by McQueen, Marsh, Taylor, Fritz, and Carter [22]. In this appendix a simplified form of the equation of state is described, which makes possible explicit calculations of thermodynamic variables, at the expense of accuracy. The equation of state is assumed to have the Mie-Gruneisen form

$$p = G \rho_0 I + g(\rho) \quad , \tag{1}$$

with ρ_0 the normal density, ρ its current value, and the Gruneisen ratio, G, assumed constant. It is convenient to make use of the specific volume, V, the inverse of ρ, in the thermodynamic calculations. By combining this form with the thermodynamic identity

$$T \left(\frac{\partial p}{\partial T}\right)_V = p + \left(\frac{\partial I}{\partial V}\right)_T \quad , \tag{2}$$

it is possible to obtain a first order partial differential equation for I whose general solution has the form

$$I\, e^{GV/V_0} - \int_V^{V_0} e^{GV/V_0}\, g(v)\, dV = f(T\, e^{-G\theta}) \quad , \tag{3}$$

where

$$\theta = \frac{V_0 - V}{V_0} \quad , \tag{4}$$

represents the compression. If it is also assumed that the specific heat is constant, then

$$I = C_v T + V_0 \; e^{G\theta} \int_0^{\theta} e^{-G\theta} \; g(V) \; d\theta \quad . \tag{5}$$

It follows that the entropy is given by

$$S = S_0 + C_v \, \ell n \left(\frac{T}{T_0} \, e^{-G\theta} \right) \quad . \tag{6}$$

A form for g(V) that leads to a particularly simple expression for temperature is

$$g(V) = \left(\frac{A}{W} \right) \left(e^{W\theta} - 1 \right) \quad , \tag{7}$$

where A is the bulk modulus and W is an empirical constant. Then

$$p = G\rho_0 \, C_v \, T + \frac{A}{W - G} \left(e^{W\theta} - e^{G\theta} \right)$$

$$I = C_v \, T + \frac{A \, V_0}{W - G} \left(\frac{e^{W\theta} - 1}{W} - \frac{e^{G\theta} - 1}{G} \right) \quad . \tag{8}$$

For a variety of materials W is about 5 and G is near 2. Taylor [23] has measured the release temperature of copper shocked to 150 GPa, and finds T ~ 1350 K, the melting point. He cites data by McQueen and Marsh [24] indicating that the melting point is just attained for a shock pressure of 140 GPa, for which $\theta = 0.3$. With G = 2, W = 5.1, and the known data, A = 139 GPa, C_v = 0.37 KJ/Kg, and $\theta = 0.3$, the approximation cited leads to a shock pressure of 140 GPa, a temperature rise of 2328°K at the shock, and an adiabatic release to 1341 K. This is in good agreement with Taylor's measurement. In general, however, one should not expect accuracy of better than 10% with this approximate theory and should not stray far from known data. The intent here is not to suggest an alternative to the standard approaches, but a useful approximation.

REFERENCES

1. R. C. Jensen, E. J. Blommer, and B. Brown in: 7th Symposium on Detonation J. M. Short, Ed. (Annapolis, MD, June 16-19, 1981).
2. L. G. Green, E. James, E. L. Lee, E. S. Chambers, C. M. Tarver, C. Westmorland, A. M. Weston, and B. Brown in: 7th Symposium on Detonation, J. M. Short, Ed. (Annapolis, MD, June 16-19, 1981).
3. J. D. Jacobsen and R. R. Karpp in: 2nd Propulsion Systems Hazards Meeting (Naval Weapons Center, China Lake, CA, April 19-21, 1982).

4. L. Seaman, D. R. Curran, and D. A. Shockey, J.A.P. 47, 11 (1976).
5. J. K. Dienes in: Colloque Internationale du CNRS No. 351, J.-P. Boehler, Ed. (Villard-de-Lans, France, June 21-24, 1983).
6. J. K. Dienes in: 2nd Propulsion Systems Hazards Meeting, (Naval Weapons Center, China Lake, CA, April 19-21, 1982).
7. R. N. Rogers, Thermochimica Acta, 11, 131-139 (1975).
8. D. A. Frank-Kamenetskii, Acta Physicochem. USSR, 10, 365 (1939).
9. R. B. Frey in: Seventh Symposium on Detonation (Annapolis, MD, June 16-19, 1981).
10. Y. L. Bai, J. Mech, Phys. Solids, 30, 4 (1982).
11. T. R. Gibbs and A. Popolato, LASL Explosive Property Data (University of California Press, Berkeley, 1980).
12. W. Hermann and J. W. Nunziato in: Dynamic Response of Materials to Intense Implosive Loading, P. C. Chou and A. K. Hopkins, eds. (Air Force Materials Laboratory, Wright Patterson AFB, OH 1972) pp. 123-281.
13. M. L. Kachanov, Mech of Materials, 1, 1 (1982).
14. B. E. Cummings and M. L. Williams in: Mechanical Behavior of Materials (Kyoto University, Kyoto, Japan, August 21-24, 1974).
15. J. K. Dienes and L. G. Margolin in: 21st U.S. Symposium on Rock Mechanics (Rolla, MO, June 1980).
16. J. K. Dienes, Acta Mechanica, 32, 217-232 (1979).
17. W. Noll, J. Rat'l Mech. Anal. 4 (1955).
18. J. K. Dienes in: 22nd U.S. Symposium on Rock Mechanics, H. H. Einstein, Ed. (Boston, MA, June 1981).
19. J. K. Dienes in: 19th U.S. Symposium on Rock Mechanics, Y. S. Kim, Ed. (Stateline, NV, May 1978).
20. J. K. Dienes in: 23rd U.S. Symposium on Rock Mechanics, R. E. Goodman and F. E. Henze, eds. (Berkeley, CA, August 1982).
21. J. M. Walsh and R. H. Christian, Phys. Rev. 97, 1544 (1955).
22. R. G. McQueen, S. P. Marsh, J. W. Taylor, J. N. Fritz, and W. J. Carter in: High-Velocity Impact Phenomena, R. Kinslow, ed. (Academic Press, NY, 1970).
23. J. W. Taylor, J.A.P. 34, 9 (1963).
24. R. G. McQueen and S. P. Marsh, J.A.P. 31, 7 (1960).